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CONSTRUCTION OF G −OPTIMAL MULTI-FACTOR MIXTURE EXPERIMENTS USING FRACTIONAL FACTORIAL DESIGNS

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ABSTRACT

Experiments in which response is a function of proportions of components present in the mixture and not of the total amount of mixture, are called mixture experiments. In practice, there do occur experimental situations in which the experimenter is interested in studying the effect of mixtures of two or more independent factors simultaneously. Such types of experiments are known as multi-factor mixture experiments. So an alternative method is proposed to construct the multi-factor mixture experiments using fractional factorial design as an initial design obtained by the minimum aberration criteria.

KEYWORDS: Mixture Experiments, Fractional Factorial Design, G-Efficiency, Multi-Factor Experiments, Quadratic Model, etc

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INTRODUCTION

In mixture experiment the response to a mixture of q components is a function of the proportions x_i $(i = 1,2, \dots \dots, q)$ of components in the mixture. The proportions x_i must satisfy the constrains

$$0 \le x_i \le 1$$

and

$$\sum_{i=1}^{q} x_i = 1$$

Mixture experiments introduced by Scheffe (1958) have a somewhat limited scope of practical utility in the sense that these allow investigation of only one factor at a time. The components of any mixture experiment have to be some or other kind of single factor. For instance, a crop mixture experiment requires that the components must be some or the other crop. Similarly, fertilizer trials can be studied as mixture experiments if we regard different types of fertilizers as their components.

There do occur experimental situations where proportions of components of two or more independent factor are to be tested. These types of experiments are called multi-factor mixture experiments. Designs and models for such multi-factor experiments were suggested by Lambrakis (1968) and Nigam (1973). If multi-factor mixture experiments consisting of two factor X and Z where the first factor (X) has p −components and second factor (Z) has q − components, then this two factor mixture will have the following constraints

$$0 \le x_i \le 1 \qquad \sum_{i=1}^{p} x_i = 1$$

and

$0 \leq z_i \leq 1 \qquad \sum_{j=1}^{q} z_j = 1$

In general, for n −factor mixture experiment, if x_{ij} represents the j^{th} component of i^{th} factor, where the i^{th} factor having p_i components, then the restrictions are

$0 \leq x_{ij} \leq 1 \qquad i = 1,2, \dots \dots, n$

$j = 1,2, \dots \dots, p_i$

$\sum_{i=1}^{p_i} x_{ij} = 1 \qquad \forall\, i = 1,2 \dots \dots, n$

Such experimental situations are known as multi-factor mixture experiments. Nigam (1973) derived the quadratic model for two-factor mixture experiments and gave the procedure of obtaining block designs for multi-factor mixture experiments. This procedure demand that for multi-factor mixture experiments the design should be so selected that at each of the combinations of components of one factor, all combinations of components of the other factors must occur. Kumari and Mittal (1986) gave a method of construction of two factor mixture experiments. It has been assumed that the experimenters are interested in small region around a main point of interest within the factor space of the components. They have considered following linear model for two factor experiments when the experimental region is restricted around a specified point. Murthy and Murty (1989) have given two methods of construction of designs for multi-factor mixture experiments involving only two factors. They obtained the designs by transformations of symmetric factorial designs. Prescott (2000) has given some illustrative examples of projections of response surface designs into constrained mixture simplex. Alam (2010) extended the method of construction of designs for single factor mixture experiments given by Prescott (2000) for the construction of multi-factor mixture experiments.

In the present study, an alternative method is proposed to construct the multi-factor mixture experiments. The method proposed by Alam (2010) is altered by using regular fractional factorial designs as initial design in place of symmetric factorial designs. Hinkelmann and Kempthorne (1994) discussed about the regular fractional factorial designs. Accordingly, a 2^{-m} th distinct combinations will be referred to as a 2^{n-m} regular fractional factorial design. Resolution [Box and Hunter 1961] and its refinement, minimum aberration [Fries and Hunter 1980] are commonly used criteria for selecting regular 2^{n-m} designs. Cheng, Steinberg and Sun (1999) found that these criteria give good measures of the estimation capacity of a fractional design. Due to this reason, designs obtained by the minimum aberration are used as initial design to construct multi-factor mixture experiments.

METHOD AND CONSTRUCTION

To construct the designs for n −factor mixture experiments, where the i^{th} factor is having p_i components, following steps may be followed.

Step 1: Take regular fractional factorial design $\boldsymbol{Z}$ (unconstrained design) in $\sum_{i=1}^{n} p_i$ factors. The first p_1 columns of $\boldsymbol{Z}$ will be projected to construct the mixture component of the first factor, second p_2 columns will be projected to construct the mixture component of the second factor and so on. In other words, $\boldsymbol{Z}$ is projected into a constrained mixture region. For this a projection matrix $\boldsymbol{P}$ is needed i.e.

$\boldsymbol{Z_n} = \boldsymbol{ZP}$

such that the constrained design $\boldsymbol{Z_n}$ satisfies constrained arising from the mixture experiments. Here

$$\boldsymbol{P} = \begin{bmatrix} \boldsymbol{P_1} & \boldsymbol{0} & \dots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{P_2} & \dots & \boldsymbol{0} \\ \dots & \dots & \dots & \dots \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{P_n} \end{bmatrix}_{\sum_{i=1}^{n} p_i \times \sum_{i=1}^{n} p_i} \qquad \forall\, i = 1,2, \dots \dots, n$$

In matrix notation

$$\boldsymbol{P_i} = \boldsymbol{I_i} - \boldsymbol{1}_i\left(\boldsymbol{1}_i'\boldsymbol{1}_i\right)^{-1}\boldsymbol{1}_i'$$

$$= \boldsymbol{I_i} - \frac{\boldsymbol{1}}{\boldsymbol{p_i}}\left(\boldsymbol{1}_i\boldsymbol{1}_i'\right)$$

Step 2: Now consider the u^{th} run of $\boldsymbol{Z}$ such that

$$z_{iju} = \frac{x_{iju} - x_{0i}}{\alpha_i} \qquad u = 1,2, \dots, N$$

$$j = 1,2, \dots, p_i$$

$$i = 1,2, \dots, n$$

where α_i is the scaling constant for the i^{th} factor required to ensure that all runs lie within mixture region. In general α_i lies between 0 to $\frac{1}{p_i}$.

In matrix notation

$$\boldsymbol{X_i} = \alpha_i \times \boldsymbol{Z_{p_i}} + \frac{\boldsymbol{1}}{\boldsymbol{p_i}} \times \boldsymbol{J_i}$$

where X_i is the design point for the i^{th} factor, $\boldsymbol{Z_{p_i}}$ is the i^{th} partition of $\boldsymbol{Z_p}$, $\boldsymbol{J_i}$ is a matrix of order $N \times p_i$ with element 1.

For example, consider the mixture experiment which consists of two factors, where both factors are with three components ($p_1 = p_2 = 3$). For this 2^{2+2} fractional factorial arrangements obtained through method of minimum aberration are required. Let the design matrix $\boldsymbol{Z}$ is given by

Table 1

		-1	**-1**	**-1**	**-1**	**-1**	**-1**	
		-1	-1	-1	-1	-1	1	
		-1	1	-1	-1	-1	1	
		-1	1	-1	-1	-1	-1	
		1	-1	1	-1	-1	1	
		1	-1	1	-1	-1	-1	
		1	1	1	-1	-1	-1	
		1	1	1	-1	-1	1	
		-1	-1	-1	1	-1	1	
		1	-1	-1	1	-1	-1	
		-1	1	-1	1	-1	-1	
		1	1	-1	1	-1	1	
		-1	-1	1	1	-1	-1	
		1	-1	1	1	-1	1	
		-1	1	1	1	-1	1	
		1	1	1	1	-1	-1	

Table 1: Contd.,								
Z=		-1	-1	-1	-1	1	1	
		1	-1	-1	-1	1	-1	
		-1	1	-1	-1	1	-1	
		1	1	-1	-1	1	1	
		-1	-1	1	-1	1	-1	
		1	-1	1	-1	1	1	
		-1	1	1	-1	1	1	
		1	1	1	-1	1	-1	
		-1	-1	-1	1	1	-1	
		1	-1	-1	1	1	1	
		-1	1	-1	1	1	1	
		1	1	-1	1	1	-1	
		-1	-1	1	1	1	1	
		1	-1	1	1	1	-1	
		-1	1	1	1	1	-1	
		1	1	1	1	1	1	

To project $\boldsymbol{Z}$ into a constrained mixture region, it is require a projection matrix $\boldsymbol{P}$ to give $\boldsymbol{Z_p} = \boldsymbol{ZP}$, such that the constrained design $\boldsymbol{Z_p}$ satisfies the constraints arising from mixture experiment. Here

$$P = \begin{bmatrix} 0.67 & -0.33 & -0.33 & 0 & 0 & 0 \\ -0.33 & 0.67 & -0.33 & 0 & 0 & 0 \\ -0.33 & -0.33 & 0.67 & 0.67 & -0.33 & -0.33 \\ 0 & 0 & 0 & -0.33 & 0.67 & -0.33 \\ 0 & 0 & 0 & -0.33 & -0.33 & 0.67 \end{bmatrix}$$

and scaling constants α_i are chosen in such a way that in the resulting design each component lie between 0 and 1. By taking $\alpha_1 = \alpha_2 = \frac{1}{6}$ all the points are within the mixture simplex region and the resulting mixture design matrix is given by

Table 2

x_{11}	x_{12}	x_{13}	x_{21}	x_{22}	x_{23}
0.3333	0.3333	0.3333	0.3333	0.3333	0.3333
0.3333	0.3333	0.3333	0.2222	0.2222	0.5556
0.2222	0.5556	0.2222	0.2222	0.2222	0.5556
0.2222	0.5556	0.2222	0.3333	0.3333	0.3333
0.4444	0.1111	0.4444	0.2222	0.2222	0.5556
0.4444	0.1111	0.4444	0.3333	0.3333	0.3333
0.3333	0.3333	0.3333	0.3333	0.3333	0.3333
0.3333	0.3333	0.3333	0.2222	0.2222	0.5556
0.3333	0.3333	0.3333	0.4444	0.1111	0.4444
0.5556	0.2222	0.2222	0.5556	0.2222	0.2222
0.2222	0.5556	0.2222	0.5556	0.2222	0.2222
0.4444	0.4444	0.1111	0.4444	0.1111	0.4444
0.2222	0.2222	0.5556	0.5556	0.2222	0.2222
0.4444	0.1111	0.4444	0.4444	0.1111	0.4444
0.1111	0.4444	0.4444	0.4444	0.1111	0.4444
0.3333	0.3333	0.3333	0.5556	0.2222	0.2222
0.3333	0.3333	0.3333	0.1111	0.4444	0.4444
0.5556	0.2222	0.2222	0.2222	0.5556	0.2222
0.2222	0.5556	0.2222	0.2222	0.5556	0.2222
0.4444	0.4444	0.1111	0.1111	0.4444	0.4444

Table 2: Contd.,					
0.2222	0.2222	0.5556	0.2222	0.5556	0.2222
0.4444	0.1111	0.4444	0.1111	0.4444	0.4444
0.1111	0.4444	0.4444	0.1111	0.4444	0.4444
0.3333	0.3333	0.3333	0.2222	0.5556	0.2222
0.3333	0.3333	0.3333	0.4444	0.4444	0.1111
0.5556	0.2222	0.2222	0.3333	0.3333	0.3333
0.2222	0.5556	0.2222	0.3333	0.3333	0.3333
0.4444	0.4444	0.1111	0.4444	0.4444	0.1111
0.2222	0.2222	0.5556	0.3333	0.3333	0.3333
0.4444	0.1111	0.4444	0.4444	0.4444	0.1111
0.1111	0.4444	0.4444	0.4444	0.4444	0.1111
0.3333	0.3333	0.3333	0.3333	0.3333	0.3333

Wheelar (1972) suggested that any design with G-efficiency ≥ 50% could be "good" design for practical purpose and showed that pursuit of higher efficiencies is not generally justified in practice. Therefore, the efficiency of above design is given by

$$G - efficiency = 0.6340$$

The results are proposed by SAS and summarized in Table which gives the G-efficiency of multifactor mixture design at different number of factors and their components procured by above mentioned method.

Table 3: G-efficiencies of Multi—Factor Mixture Experiments for $n \leq 3$ and $p_i \leq 3$

Number of Factor	Component for Each Factor	G-Efficiency
2	2,2 2,3 3,3	0.9905 0.6308 0.6340
3	2,2,2 2,2,3 2,3,3 3,3,3	0.5265 0.6021 0.6593 0.7141

CONCLUSIONS AND DISCUSSIONS

In agriculture experiments, the behavior of different ingredients in generally quadratic in nature, therefore, designs for multi-factor mixture experiments has been obtained so as to fit the second order response surface model. A method for obtaining unique parameter estimates for the second order model for multi-factor mixture experiments has been developed. Method has been developed to construct designs with fewer numbers of runs so as to fit the second order mixture models and the design constructed has been evaluated with G-efficiency. Method of construction is based on projection of fractional factorial design as initial design. It is found that the constructed mixture design with G-efficiencies around 50% which could be good design for practical purposes. The G-efficiencies procured by the method increases as the minor components increases.

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